Koch, Kristine

From: Allen, Elizabeth
Sent: Tuesday, November 25, 2014 6:26 PM
To: John Toll; Suzanne Replinger; Koch, Kristine; James McKenna; Jennifer Woronets
Subject: FW: bioaccumulation models for additional PCDD/F congeners of interest

John/Suzanne,

When we discussed the values shown in the attached table a few weeks ago, I mentioned that we'd need references for the values presented, Kow and the invertebrate and vertebrate Km values. Of particular curiosity is the Kow for 1,2,3,7,8-PeCDD. It's a lot lower than most of the values we've seen in the literature, and lower than the recommended value for TCDD, which seems counterintuitive given that PeCDD should be less water soluble given the higher chlorination. Can you provide some insight into this?

Thanks

Elizabeth

From: John Toll [mailto:JohnT@windwardenv.com]
Sent: Friday, August 22, 2014 5:43 PM
To: James McKenna
Cc: Bob Wyatt (rjw@nwnatural.com); Jennifer Worenets (jworonets@anchorqea.com); Patty Dost (pdost@pearllegalgroup.com)
Subject: bioaccumulation models for additional PCDD/F congeners of interest

Hi Jim,

Windward has completed the bioaccumulation model for the additional PCDD/F congeners of interest (1,2,3,4,7,8-HexaCDF; 1,2,3,6,7,8-HexaCDD; 1,2,3,7,8-PentaCDD; 2,3,7,8-TCDF and 2,3,7,8-TCDD). This was a lot of work in a very short time, but we are confident that the models are good. The following table shows the congener-specific parameters for the calibrated congener models, and the model performance statistics (SPAFs).

Summary of selected parameter values for dioxin/furan congener bioaccumulation models and calibrated model performance

DF Congener	Parameter	Unit	Nominal Value	Range / Distribution	Selected Value	Notes	Calibrated Model Performance
1,2,3,4,7,8-HexaCDF	Sediment SWAC	µg/kg	0.00271	-	0.00271		

	Water concentration - site	ng/L	1.10E-05	-	1.10E-05		Fish SPAFs: CAR = 1.3 (-) SMB = 1.7 (+)
	Water concentration - bkgd	ng/L	7.23E-06	-	-	used for PRGs only	
	log K_{OW}	kg/L	7.66	6.92 - 7.92	7.0		
	Invertebrate K_M	1/day	0	none	0		
	Fish K_M	1/day	no info	no info	0.02		
1,2,3,6,7,8-HexaCDD	Sediment SWAC	µg/kg	0.0766	-	0.0766		Fish SPAFs: CAR = 2.3 (-) SMB = 1.5 (+)
	Water concentration - site	ng/L	2.43E-05	-	2.43E-05		
	Water concentration - bkgd	ng/L	1.61E-05	-	-	used for PRGs only	
	log K_{OW}	kg/L	7.74	7.58 - 9.13	7.74		
	Invertebrate K_M	1/day	0	none	0		
	Fish K_M	1/day	0.04	0 - 0.4	0.08		
1,2,3,7,8-PentaCDD	Sediment SWAC	µg/kg	0.00025	-	0.00025		Fish SPAFs: CAR = 1.9 (-) SMB = 1.4 (+)
	Water concentration - site	ng/L	6.91E-06	-	6.91E-06		
	Water concentration - bkgd	ng/L	2.11E-06	-	-	used for PRGs only	
	log K_{OW}	kg/L	7.06	6.49 - 7.56	6.7		
	Invertebrate K_M	1/day	0	none	0		
	Fish K_M	1/day	0.02	0 - 0.2	0.01		
2,3,7,8-TetraCDF	Sediment SWAC	µg/kg	0.0168	-	0.0168		Fish SPAFs: CAR = 1.1 (-) SMB = 1.2 (+)
	Water concentration - site	ng/L	7.83E-06	-	7.83E-06		
	Water concentration - bkgd	ng/L	3.75E-06	-	-	used for PRGs only	
	log K_{OW}	kg/L	6.3	5.82 - 7.7	7.5		
	Invertebrate K_M	1/day	0	none	0		
	Fish K_M	1/day	0.04	0.04 - 0.2	0.1		
2,3,7,8-TetraCDD	Sediment SWAC	µg/kg	0.0001	-	0.0001		

	Water concentration - site	ng/L	1.25E-05	-	1.25E-05		
	Water concentration - bkgd	ng/L	3.24E-06	-	-	used for PRGs only	Fish SPAFs: CAR = 1.4 (+) SMB = 1.9 (-)
	log K_{OW}	kg/L	6.38	5.38 - 8.93	6.9		
	Invertebrate K_M	1/day	0	none	0		
	Fish K_M (other spp)	1/day	0.007	0.007 - 0.024	0.007		
	Fish K_M (carp)	1/day	0.0016	0.0016 - 0.056	0.0016		

A SPAF of 1 means that the model-predicted tissue concentration exactly equals the sample average tissue concentration. A SPAF of 2 means that the model predicts the sample average with a factor of 2, etc. Within a factor of 2 is an excellent agreement (because keep in mind that the sample average tissue concentrations that we compare to are also uncertain estimates of the true mean). We calibrated to carp and smallmouth bass because these are target species for the HHRA with robust datasets. You'll see that all SPAFs for all congeners of interest are within a factor of 2. If we'd have had more time we'd have done more testing of model fit, (e.g., evaluating the consistency of calibrations across congeners in greater depth). But we're very happy with the calibrations and we believe that the models are suitable and ready to use for calculating congener-specific PRGs.

In addition to the bioaccumulation modeling there is another step that is necessary to calculate sediment PRGs for individual PCDD/F congeners. That step is developing statistical regression models between individual congener concentration in fish tissue and the TEQ concentration in fish tissue.

Once we calculate the regression models, we can convert the TEQ target tissue concentration into an individual congener target tissue concentration. The individual congener target tissue concentrations are the inputs to the bioaccumulation model, which is run backward to calculate the PRGs.

We've had a very unfortunate problem come up that has slowed down our work on the statistical regressions. Our statistician lives in the Methow Valley. A couple weeks ago she lost her house in the fires, along with virtually all of their possessions. Everyone's okay, they have temporary housing, and they've already turned their attention to rebuilding, but she's been unable to work.

Understanding EPA's request to have as much of this draft work completed by close of business today, we attempted a simpler and weaker approach to calculating the tissue TEQ to tissue congener relationships, but it hasn't worked. We are getting predictions that are not consistent with the empirical data. We can fix this problem, but we need a little more time. We think it's going to be the latter part of next week before we'll have defensible model inputs (target tissue concentrations for individual congeners). We need to get those inputs right before we can get defensible PRGs out of the bioaccumulation models. So, the bioaccumulation models are done, but we need a little more time to generate the model inputs that we need to calculate PRGs.

Let me know please if you have any questions or concerns.

John